Introducing Computational Science in the Curriculum – Part 3

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Creating a Conceptual Model

- Start with a topic that everyone can relate to
- Discuss all of the conditions that will affect the system
- Discuss simplification into a model
- Introduce modeling terminology

First Modeling Exercise

- Model of the time it takes to get from your house to a place of work using alternate routes
- Possible Objectives
  - Minimize the time it takes
  - Avoid traffic congestion
  - Avoid freeways (old car)
  - Go by a friends house, restaurant, etc.

Conceptual Model

- List all **variables** of importance
- Define **cause and effect** relationships
  - From scientific evidence or theories
  - From physical “laws”
  - From our own ideas
- Estimate nature of the relationship, form of the relationship, and quantitative estimate

Weather and Traffic

Weather Condition	Impact on Traffic Flow
Clear skies, no wind	
Light rain	
Heavy rain	
Light snow	
Heavy snow	
Heavy snow and blowing, poor visibility	
Freezing rain	
Other?	

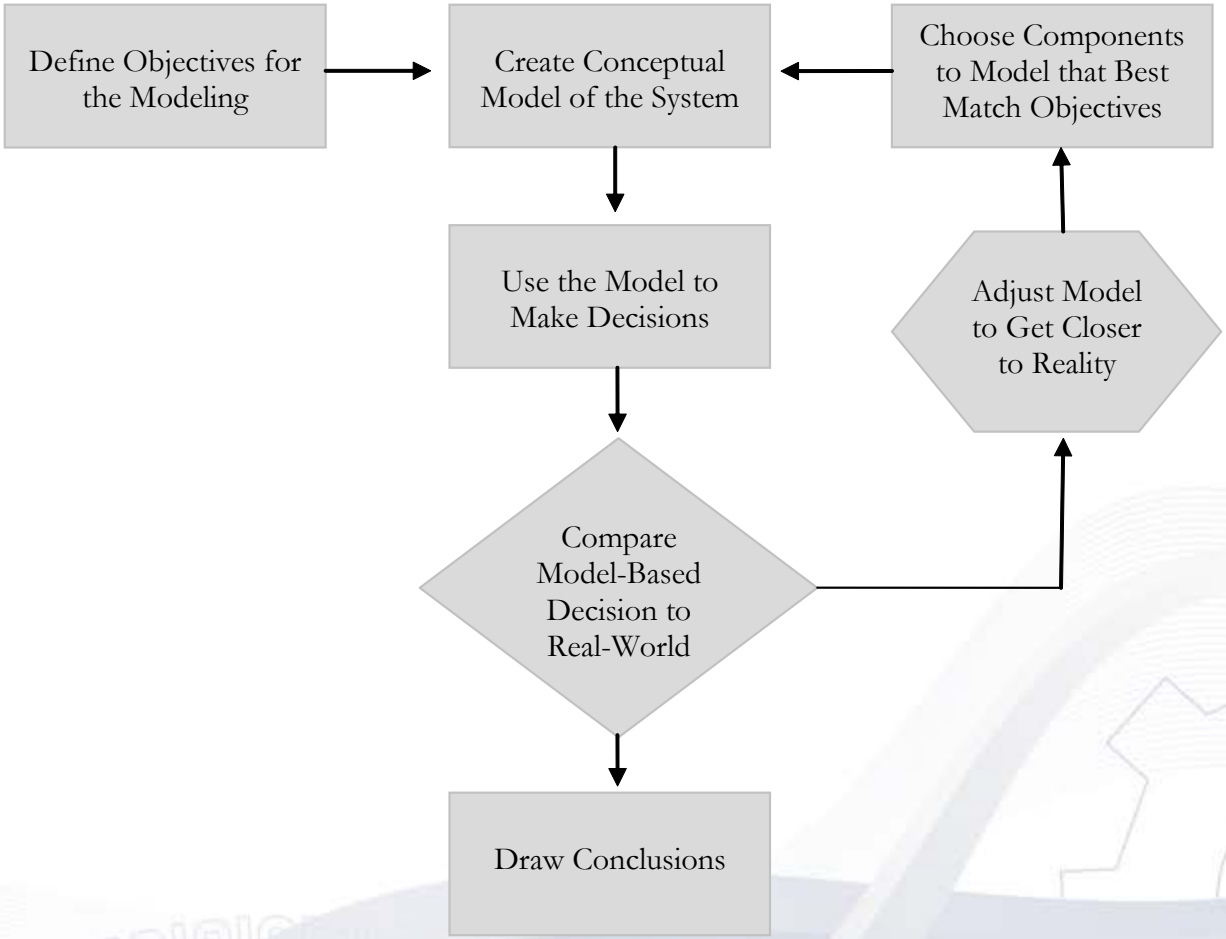
More Modeling Ideas

- Assess the **accuracy** of our model
  - How close does it come to the real answer?
  - How would we measure this?
- Simplify the model – eliminate some variables from consideration
  - Decide which conditions represent the “majority” of cases
  - Leave out other conditions to be modeled at a later time

Still More Ideas

- Hold some **variables** constant for a range of forecasts
  - Sometimes referred to as model **parameters**
  - Test the **sensitivity** of the results to changes in the values of the parameters
- **Verify** whether the calculations are done correctly
  - Is the code correct? Is the computer algorithm being used appropriately in the calculation?
- **Validate** the model as accurate
  - Compare the model results with experimental data

Figure 2: The Modeling and Inquiry Process



Conceptual Traffic Model

- Assuming we want to minimize the time it takes us to go from home to work, what should be the conceptual components of our traffic model?
- Open file trafficmodel.pdf to see the assignment
- Examine the code – traffic1b (discuss)
- Run the model from the website using different values for red light time
- Which route is preferred and when?

Optional Extension

- Focus on the nature of the traffic flow versus congestion relationship
  - Relationship is not linear as congestion increases
  - Potential differences in results if highly congested conditions exist
- Opportunity to discuss the model limitations
  - Forecasting with assumptions that are violated by the conditions
  - Forecasting beyond experimental data
  - Passing a critical point where physical conditions or behaviors change significantly

Extending This Approach

- The same approach can be used for modeling examples from a wide range of science and engineering phenomena
  - Conceptual model of the system
  - Examine a current model and define its implicit and explicit assumptions
  - Use the model to gain insights about the system
  - Learn about additions that can relax assumptions
  - Connect with programming and algorithm applications
  - Verify and validate the model

Non-Linear Phenomena

- Many phenomena are not amenable to representation by linear models
- Non-linear models can be applied
- Must understand the form of the relationship from experimental data

Examples of Non-linear Equations

- Logarithmic
- Quadratic
- Exponential
- Polynomials

Quadratic Equations

- Basic form

  f(x) = a * x2 +b*x +c

- Visualizing a quadratic function
  - **http://www.shodor.org/interactivate/activities/FunctionFlyer/**

- Try this equation

  $f(x) = 2x^2 + 10x + 6$

  Use the applet to understand the effect of changing the coefficients on function shape and location

Real-world Examples

- Bowling Ball and Car
- Other example for you to explore

  http://www.physics.umn.edu/outreach/pforce/index.html

  – Watch the Monkey and Hunter Movie

  http://physics.doane.edu/physicsvideolibrary/default.html#projectile

  – Watch movie relating to basketball toss and/or projectile truck

Observation Questions

- What are the two forces acting on the objects in the horizontal and vertical directions?
- Are the forces dependent or independent?
- If you were to graph the path of the objects, what geometric object would that path match?

Exponential Functions

- Basic form

  $f(x)= a*b^x$

- Graph in function flyer

  f(x)= 4*2^x (positive exponential)

  Change the graph limits

  – xmin=-4; xmax=15

  – ymin=-3; ymax=15

- Try **f(x)=4*2^(-1*x) (negative exponential)**

Example: Compound Interest

$$x_{t-1} = x_t e^{k}$$

where X is the value at times t and t-1

k is the growth constant

e is the base of the natural log

Traditional Expontenial Function

$$x(t) = x_0 e^{kt}$$

Solve for X at any time period given the base and the growth rate

Example Exercises

- Modeling a ball drop
- Review exercise – Quadratic Model Exercise.pdf
- Learning about recursion in programming to estimate values of a non-linear equation
- Examine the code
- Run the model
  - What is wrong with this model?